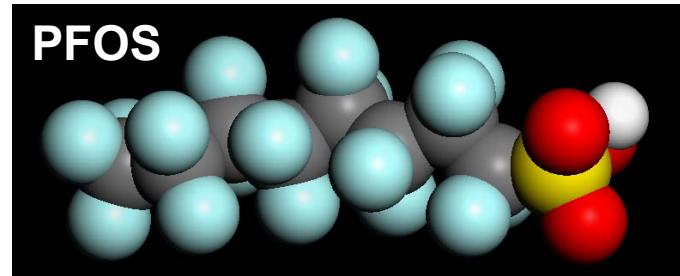
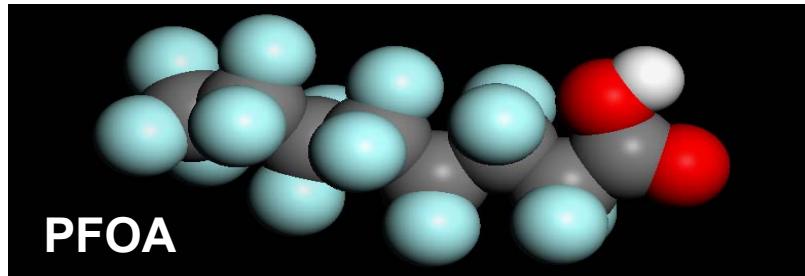


# PFOA and PFOS



Physical-Chemical Properties,  
Environmental Fate,  
Monitoring and Modeling

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# Physical–Chemical and Environmental Partitioning

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## *Physical-chemical properties*

- pKa
- Solubility
- Vapor Pressure

## *Partitioning in the environment*

- Air – water partition coefficient ( $K_{aw}$ )
- Soil – water partition coefficient ( $K_{oc}$ )
- Bioconcentration (BCF)

# Physical-chemical properties: pKa

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Chemical	pKa	Reference	Basis	Environmental significance
PFOA	3.8	Burns et al., 2008	Experiment, infinite dilution	Form in environment is combination of neutral form and anion
	2.8	Brace, 1962	Experiment, extrapolation in ethanol	Form in environment is combination of neutral form and anion
	~0	Goss, 2008	Computation with SPARC, COSMO-RS	Dominant form in environment is anion
PFOS	< 0		estimation based on acid strength	Dominant form in environment is anion

PFOSA, Me-PFOSA-AcOH and Et-PFOSA-AcOH have calculated pKa values of 6.2, 3.9 and 3.9, respectively  
Source: US Dept of Health and Human Services, ATSDR, Draft toxicological profile for perfluoroalkyls

# Physical-chemical properties: Solubility

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Chemical	Solubility (mg/L)	Reference	Basis	Environmental significance
PFOA	~ 0.025	Ellis, 2008	Experiment (unpublished)	Neutral form not soluble in water
PFO-	3600-4300 3700 9500	Kissa, 1994 Shinoda, 1972 Kauck and Diesslin, 1951	Experiment Experiment Experiment	Anion highly soluble in water
PFOS	570	3M, 2000	Experiment	Anion highly soluble in water
<b>Precursors of PFOA and/or PFOS</b>				
8-2 FTOH	0.14-0.19	Kaiser et al, 2004 Liu and Lee, 2005	Experiment Experiment	Slightly soluble in water
EtFOSE	50	3M, 1993	Experiment	
EtFOSA	< 50	Martin et al., 2006	Estimate	

# Physical-chemical properties: Vapor Pressure

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Chemical	Vapor Pressure (Pa)	Reference	Basis
PFOA	5.2 @ 27°C	Barton et al., 2008	measurement
	4.1 @ 25°C	Kaiser et al., 2005	extrapolation from measurement
APFO	0.003 @ 25°C	Barton et al., 2009	extrapolation from measurement
K+PFOS-	2.48E-08	3M, 2008	measurement
<b>Precursors of PFOA and/or PFOS</b>			
8-2 FTOH	3 @ 21°C	Krusic et al., 2005	measurement
MeFOSE	0.0020 @ 23°C	Shoeib et al., 2004	calculated from measurement
EtFOSE	0.0086 @ 23°C	Shoeib et al., 2004	calculated from measurement
EtFOSA	7.0 @ 25°C	Lei et al., 2004	measurement
MeFOSEA	0.0021 @ 23°C	Shoeib et al., 2004	calculated from measurement

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# Partitioning: Air-water partition coefficient (K<sub>aw</sub>)

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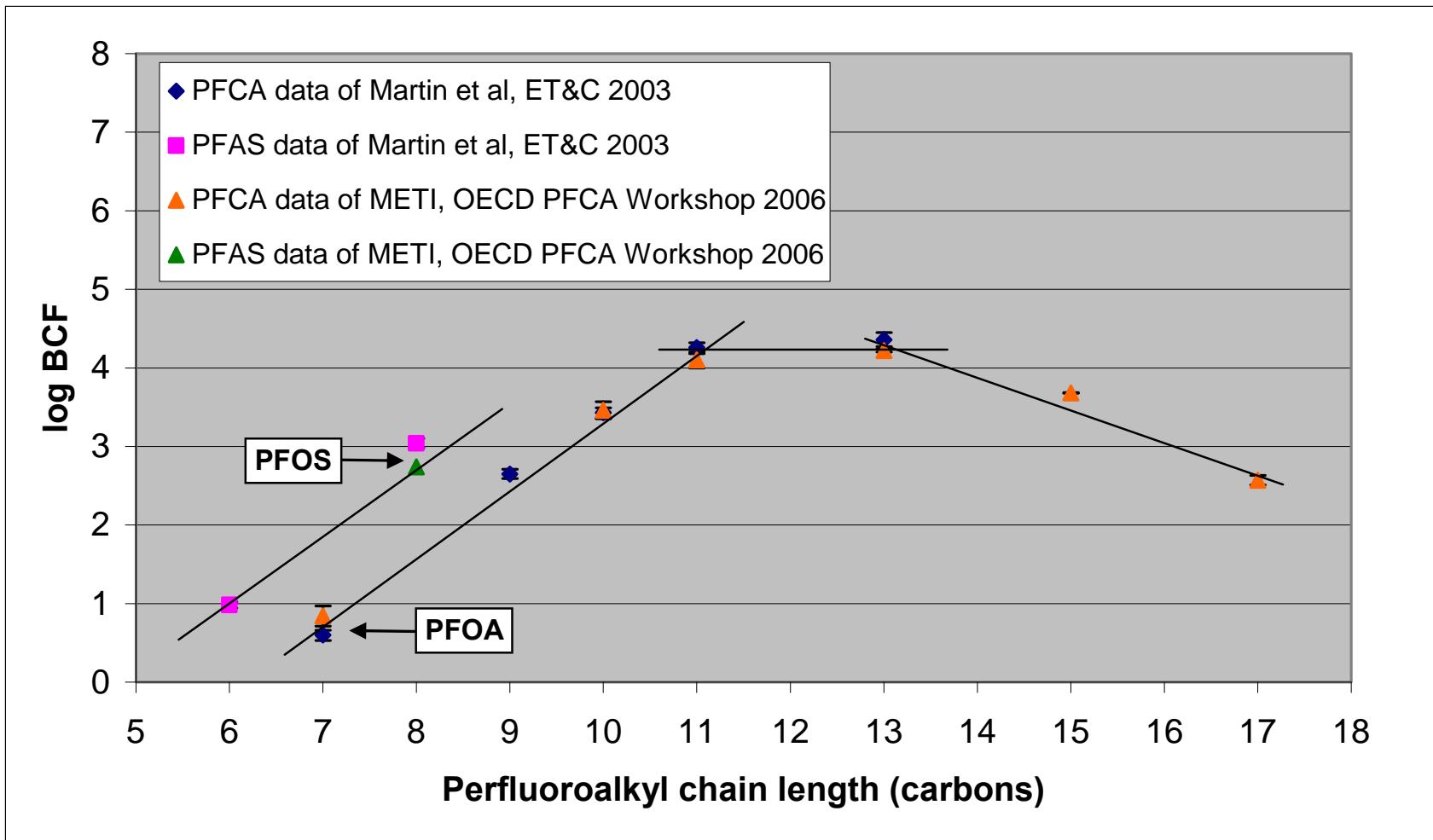
Chemical	K <sub>aw</sub>	Reference	Basis	Environmental significance
PFOA	1.02E-03 5.40E-03	Li et al., 2007 Kutsuna and Hori, 2008	measurement measurement	potential partitioning to air
PFO-	1.40E-07	Kissa, 1994 Barton et al., 2009	calculated from solubility and VP	negligible partitioning to air
PFOS	1.00E-11	3M, 2000 3M, 2008	calculated from solubility and VP	negligible partitioning to air
<b>Precursors of PFOA and/or PFOS</b>				
8-2 FTOH	3.8	Goss et al., 2006	calculated from solubility and VP	potential partitioning to air
MeFOSE	8.3E-04	Arp et al., 2006	computational chem	potential partitioning to air
EtFOSE	7.1E-03	Arp et al., 2006	computational chem	potential partitioning to air
MeFOSEA	9.1E-03	Arp et al., 2006	computational chem	potential partitioning to air

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# Partitioning: Soil-water partition coefficient (Koc)

Chemical	Koc (mL/g)	Reference	Basis	Environmental significance: mobility in soil, sediment, aquifer
PFO(A)	115 203	Higgins and Luthy, 2006 Ferrey et al., 2008	measurement measurement	high mobility medium mobility
APFO	104	Dekleva, 2003	measurement	high mobility
PFOA	~4000	Russell, unpublished	estimation based on pKa	slight mobility
PFOS	372 580	Higgins and Luthy, 2006 Ferrey et al., 2008	measurement measurement	medium mobility low mobility
<b>Precursors of PFOA and/or PFOS</b>				
8-2 FTOH	6900 3000	Liu and Lee, 2005 Swales, 2004	measurement measurement	immobile slight mobility
MeFOSAA	1290	Higgins and Luthy, 2006	measurement	low mobility
EtFOSAA	1700	Higgins and Luthy, 2006	measurement	low mobility

# Partitioning: Bioconcentration (BCF) of PFOA and PFOS in fish



# Summary of physical-chemical differences between forms of PFOA in the environment

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*Highly soluble*

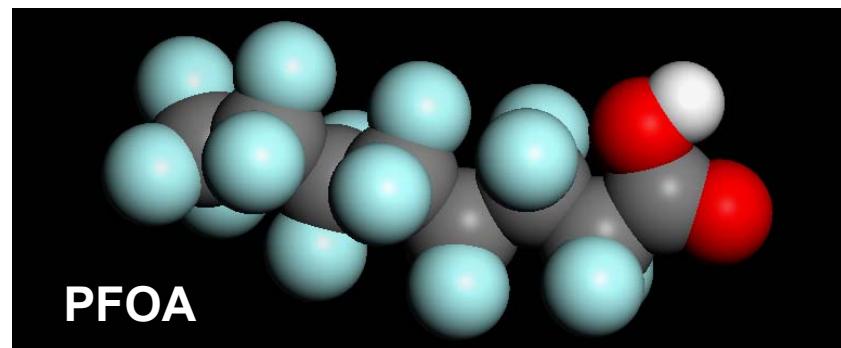
*Non-volatile*

*Poorly sorptive to soil*

*Highly insoluble*

*Some volatility*

*Highly sorptive to soil*



# Summary of physical-chemical differences between PFO(A) and PFOS in the environment

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versus  
↔



*Both anion and neutral*

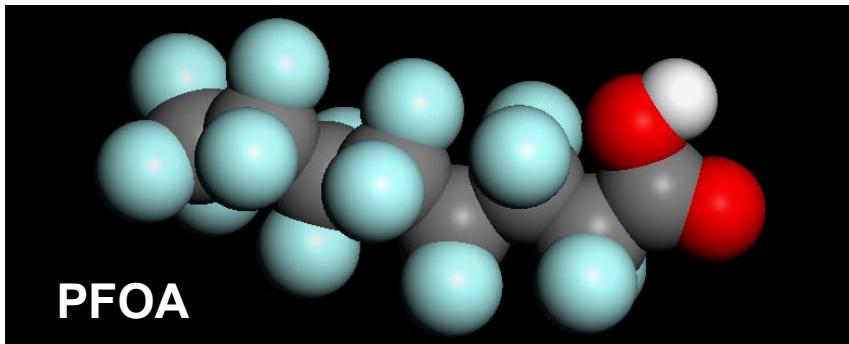
*Medium-high mobility in soil*

*No significant bioconcentration*

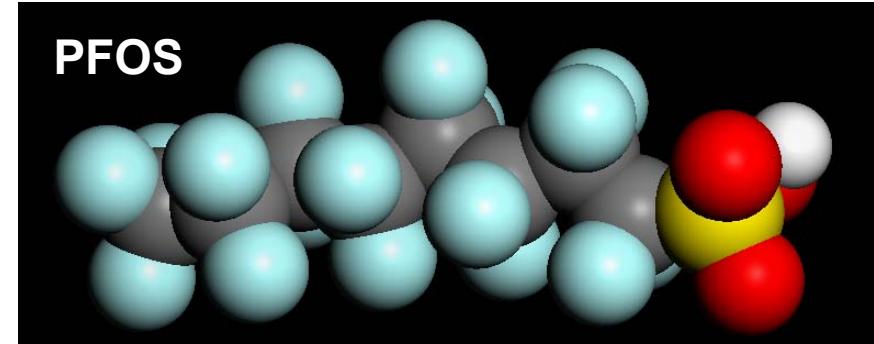
*Exclusively anion*

*Low-medium mobility in soil*

*Moderate bioconcentration*



PFOA



PFOS

# Emissions of PFOA and PFOS

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Estimated annual emissions (through year 2000)

<u>Chemical</u>	<u>Emissions</u>	<u>Reference</u>
PFOA	80 tonnes/yr	Prevedouros et al., 2006
PFOS	50 tonnes/yr	Paul et al., 2009

Current and future emissions of PFOA and PFOS are significantly lower than these historical values:

- POSF-based chemistry discontinued by 3M in 2001
- Industry commitment to reduce PFOA emissions 95% by 2010 and to work toward elimination of PFOA use by 2015

# Degradation in the Environment

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## ***Precursors of PFOA***

- Sources
- Precursor degradation pathways
- Degradation rates

## ***Precursors of PFOS***

- Sources
- Precursor degradation pathways
- Degradation rates

# Formation of PFOA in air, water and soil

Chemical	Half-life	Reference	Basis	PFOA Yield	Environmental significance
<b>Degradation of precursors and PFOA in air</b>					
8-2 FTOH	20-40 d 55-970d	Wallington et al., 2006 Yarwood et al., 2006	calculation calculation	1-10% 3-7%	moderate degradation rate in atm moderate degradation rate in atm
N-MeFOSE	2 days	D'Eon et al., 2006	estimation based on study of N-MeFBSE	>10%	rapid degradation rate in atm
N-MeFOSA	>20 d	D'Eon et al., 2006	estimation based on study of N-MeFBSE	>10%	moderate degradation rate in atm
PFO(A)	~ 130 d	Hurley et al., 2004	measurement	NA	unzipping cycle with high NOx
<b>Degradation in water</b>					
8-2 FTOH	stable	DuPont, 2004	measurement	0	hydrolysis rate is negligible
N-EtFOSE ,	40 days	3M W2783	measurement	~30-50%	aqueous photolysis
PFOS	>4, >41 yr	3M W2775, W1878	measurement	ND, <0.61%	aqueous photolysis
PFO(A)	stable				stable under normal env conditions
<b>Degradation in soil, sediment and sludge</b>					
8-2 FTOH	< 7 d (soil) < 1 d (soil) ~ 30 d (sludge)	Wang et al., 2009 Dinglasan et al., 2004 Wang et al., 2005	measurement measurement measurement	~25% ~3% ~2%	rapid degradation rate in soil rapid degradation rate in soil moderate degradation rate in sludge
N-EtFOSE ,	~ 11 d	3M E00-2252	measurement	0.16%	PFOA formed via abiotic degn of sulfinate
PFO(A)	stable	Park et al., 2009; others	measurement		stable under normal env conditions

# Formation of PFOS in air, water and soil

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Chemical	Half-life	Reference	Basis	PFOS Yield	Environmental significance
<b>Degradation of precursors in air</b>					
N-MeFOSE	2 days	D'Eon et al., 2006	estimation based on study of N-MeFBSE	>1%	rapid degradation rate in atm
N-MeFOSA	>20 d				moderate degradation rate in atm
<b>Degradation in water</b>					
N-EtFOSE	40 days	3M W2783	measurement	not detected	stable in water
PFOS	>4 - 41 yr	3M W2775, W1878	measurement	NA	stable in water
<b>Degradation in soil, sediment and sludge</b>					
N-EtFOSE	< 1 d ~11 d	Rhoads et al., 2008 3M E00-2252	measurement measurement	8% 2.4%	rapid degradation rate in sludge rapid degradation rate in sludge
PFOS	Stable	3M E01-0444	measurement	NA	stable in soil

# **Effect of reducing chain length on environmental behavior of PFCAs and PFASs**

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## Effect on physical – chemical properties

- pKa is reduced (→ more anionic species)
- Vapor pressure of precursors increases
- Vapor pressure of anions remains negligible
- Sorption of precursors and anions is reduced  
(→ more in aqueous phase)

## Effect on biota

- Bioconcentration potential is reduced
- Biopersistence is reduced

# **Environmental monitoring of PFOA and PFOS**

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## ***PFOA and PFOS in biota***

- Aquatic species
- Terrestrial species

## ***PFOA and PFOS in food crops and farm animals***

- Plant uptake
- Farm animals

# PFOA and PFOS in aquatic species



Species	Tissue	Location	PFOA (ng/g wwt)	PFOS (ng/g wwt)
<b>Invertebrates</b>				
zooplankton	whole	Florida	2.6	1.8
<i>Diporeia</i>	whole	Lake Ontario	90	280
<i>Mysis</i>	whole	Lake Ontario	2.5	13
crayfish	whole	Great Lakes	< 0.2	2.4 - 4.3
zebra mussel	soft tissue	Great Lakes	< 5	< 2 - 3.1
<b>Fish</b>				
alewife	whole	Lake Ontario	1.6	46
Atlantic croaker	whole	South Carolina	1.4	34.4
lake trout	whole	Great Lakes	0.8 - 2.4	15 - 410
pigfish	whole	Florida	< 0.5	3.1
pinfish	whole	South Carolina	< 0.5	19.4
rainbow smelt	whole	Lake Ontario	2	110
red drum	whole	South Carolina	1.2 ± 1.4	
round gobies	whole	Michigan rivers	< 2	4.1 - 21.5
slimy sculpin	whole	Lake Ontario	44	450
smallmouth bass	whole	Michigan rivers	< 2	< 2 - 41.3
spotted seatrout	whole	Florida	< 0.5	8.8

# PFOA and PFOS in terrestrial species

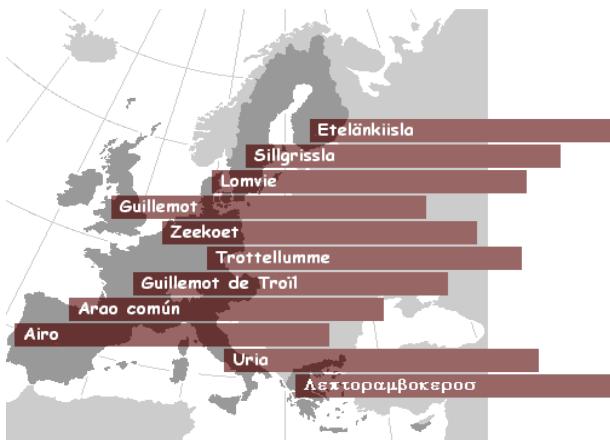


Species	Tissue	Location	PFOA (ng/g wwt)	PFOS (ng/g wwt)
<b>Birds</b>				
Northern fulmar	liver	Canada	< 2	1.3
Black-headed gull	liver	Japan	21	< 19
Common cormorant	liver	Med Sea, Italy	29 - 450	32 - 150
Snowy egret	liver	Florida	ND	43 - 413
Common loon	liver	North Carolina Mid and western US	ND ND	8.6 - 595 24 - 467
<b>Amphibians and reptiles</b>				
green frogs	liver	Michigan	< 72	< 35 - 285
Kemp's ridley sea turtle	plasma	North Carolina	3.6	39.4
Loggerhead sea turtle	plasma	Eastern USA	3.2	11
Snapping turtle	plasma	Michigan	2.5	< 1 - 169
<b>Marine Mammals</b>				
polar bears	liver	Alaska	2.4 - 3.4	537 - 793
ringed seal	liver	Canada	< 2	19



Reference: Houde et al., 2006

# Trends in PFOS and PFOA in bird eggs



Peak conc  
followed by  
decline

**TABLE 1. Concentrations of PFOS and PFOA in Guillemot Eggs (ng/g Wet Weight)**

sampling year	n	p/m <sup>a</sup>	PFOS	PFOA
1968	8	p	25	n.d. <sup>b</sup>
1971	8	m	44 (34–55)	n.d.
1973	8	p	58	n.d.
1976	8	m	162 (32–351)	n.d.
1978	8	p	169	n.d.
1981	8	m	214 (96–309)	n.d.
1983	8	p	459	n.d.
1986	8	m	233 (195–303)	n.d.
1988	8	p	485	n.d.
1991	8	m	411 (344–487)	n.d.
1993	8	p	501	n.d.
1996	8	m	528 (462–652)	n.d.
1997	8	p	1324	n.d.
1998	8	p	834	n.d.
1999	8	p	1023	n.d.
2000	8	p	871	n.d.
2001	9	m	561 (520–601)	n.d.
2003	9	m	614 (551–669)	n.d.

<sup>a</sup> p = Pool of equal aliquots of eggs from 8 individuals, m = arithmetic mean value of measurements in individual eggs. The concentration range is given in parentheses. <sup>b</sup> Not detectable at a detection limit of 3 ng/g.

# Relative plant sensitivity to PFOS in seven crops

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Plant	Relative Sensitivity (EC25, mg ai/kg)	Most sensitive endpoint
Lettuce	6.8	height
Ryegrass	7.5	shoot weight
Tomato	12	shoot weight
Onion	13	shoot weight
Alfalfa	53	shoot weight
Flax	82	shoot weight
Soybean	160	shoot weight

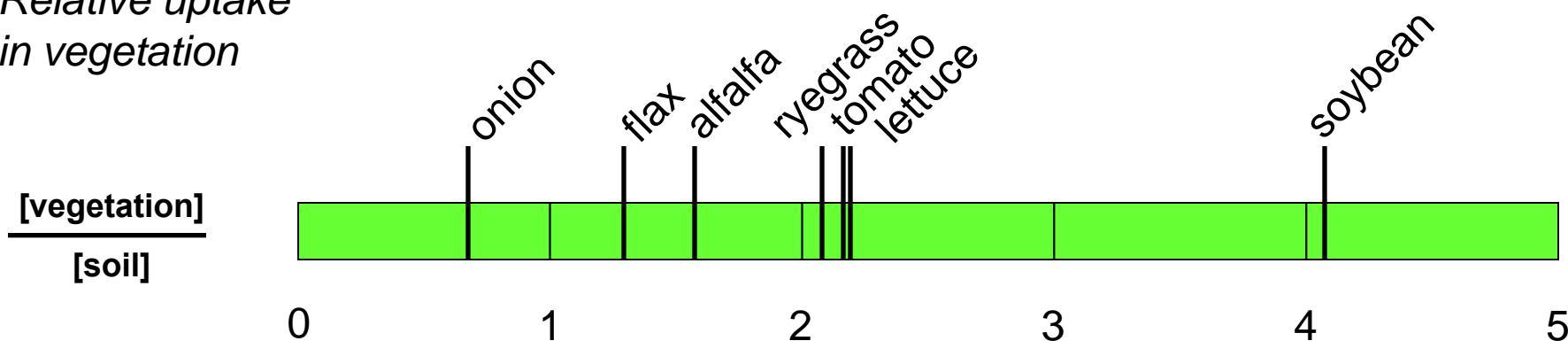
An EC25 endpoint corresponds to "slight effect, not obviously detrimental". The reported EC25 values were determined by fitting plant dose-response curves using SAS v8.

Endpoints evaluated included:

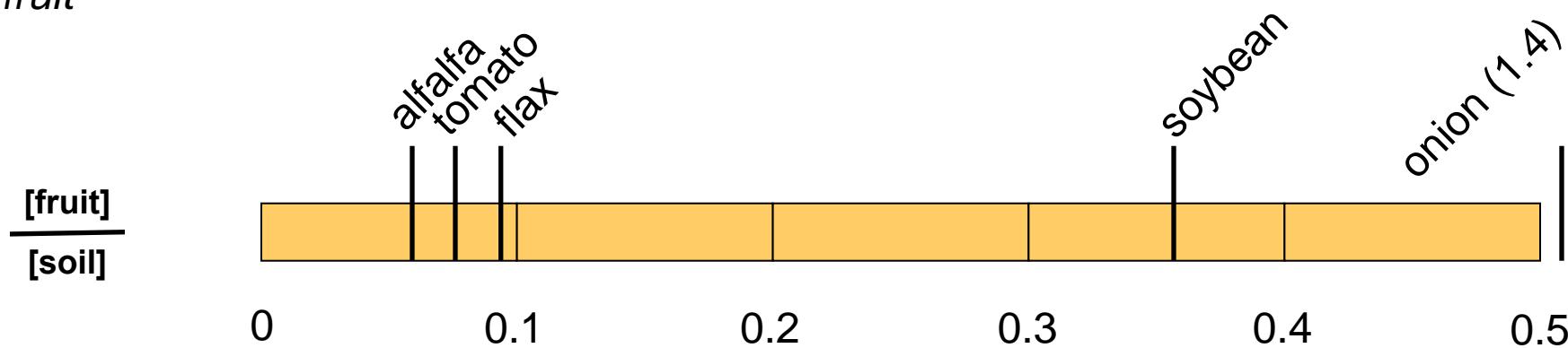
- reduction in emerged seedlings
- reduction in seedling survival
- reduction in shoot weight
- reduction in plant height

# Plant uptake of PFOS in seven crops

*Relative uptake  
in vegetation*



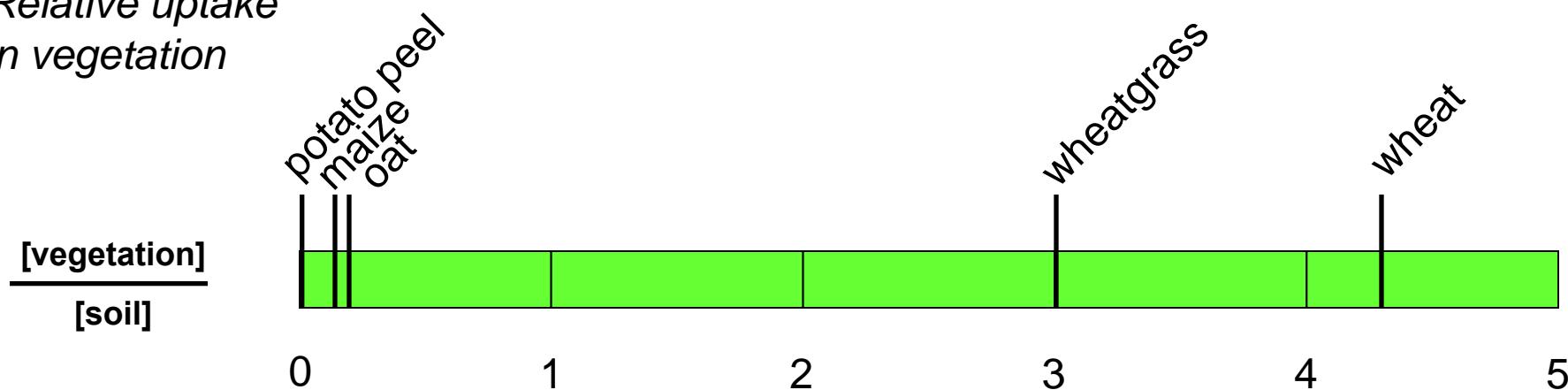
*Relative uptake  
in fruit*



Maximum plant uptake was observed at PFOS concentrations of 4-16 mg/kg in soil

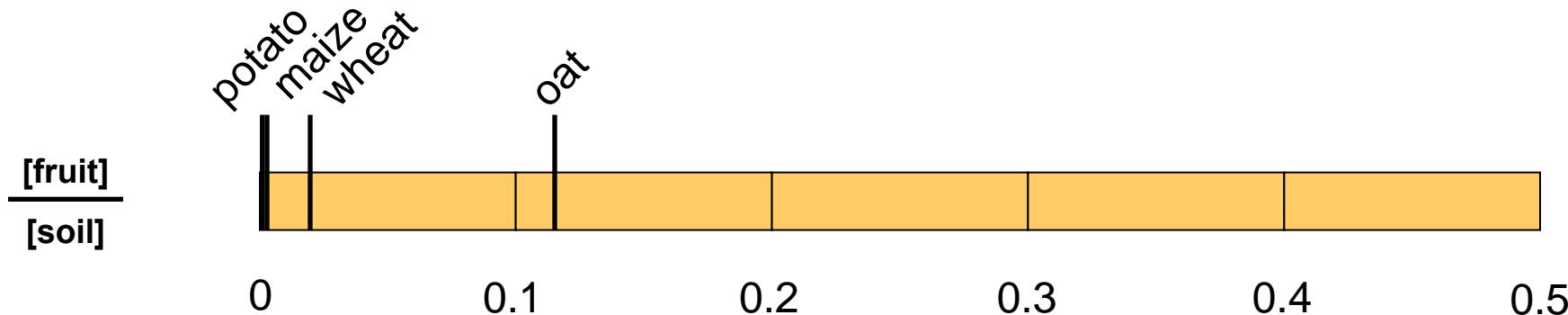
# Plant uptake of PFOA in food crops

*Relative uptake  
in vegetation*



*Relative uptake  
in fruit*

Values for PFOS are similar or up to 10X lower

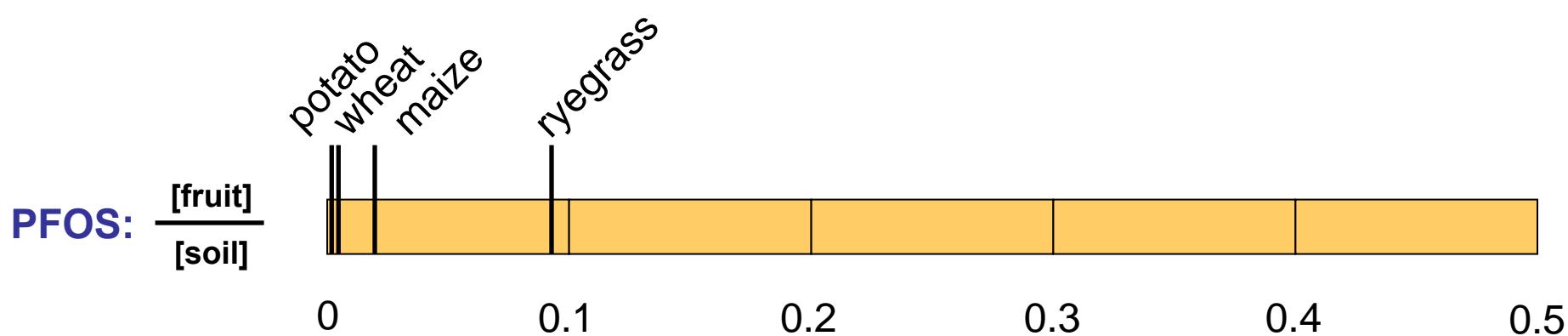
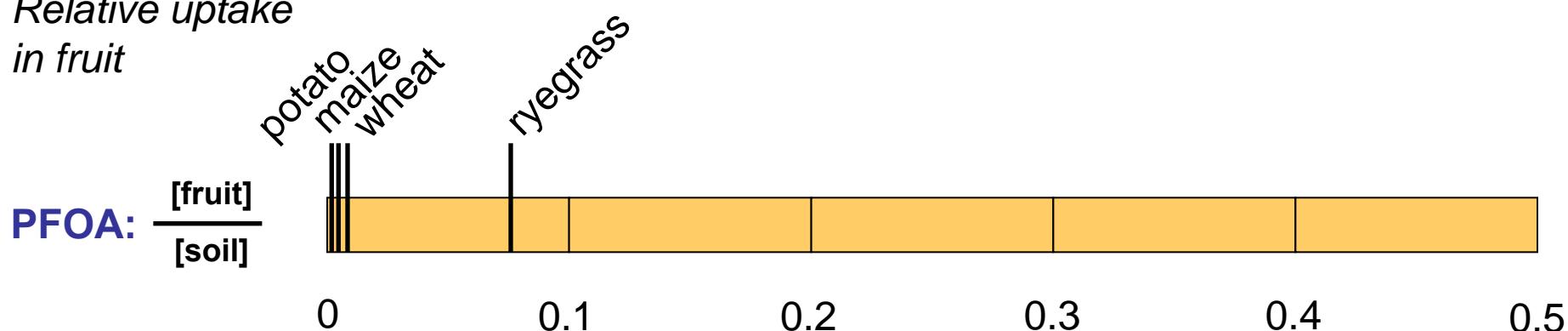


Soil concentration of PFOA or PFOS was 10 mg/kg

Reference: Stahl et al., 2008

# Plant uptake of PFOA and PFOS in food crops

Relative uptake  
in fruit



Soil concentration of PFOA or PFOS was 0.5 – 5 mg/kg

Reference: Weinfurtner, 2007

# PFOA and PFOS in livestock at a German feedlot

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## Key points

- Soil → feed → animal transfer of PFOS appears possible
- Current results are inconsistent
- Analytical methods not described
- Data not published in peer reviewed literature

Samples	PFOS ( $\mu\text{g}/\text{kg}$ )	PFOA ( $\mu\text{g}/\text{kg}$ )
<b>Soil samples</b>		
Fields	< 10 - 3100	< 10 - 130
Storage areas	25 - 12,000	< 10 - 500
<b>Feed samples</b>		
Corn silage	215	68
Grass silage	2	< 1
Feed potatoes	ND	ND
Rye	ND	ND
Water	ND	ND
<b>Animal samples</b>		
Beef cattle (blood serum)	4190 - 5070	ND
Dairy cows (blood serum)	2530 - 2650	ND
Sheep (blood serum)	10 - 34	ND
Milk	19	ND

Soil improver was applied to fields in 2006; Sludge was applied 2002 - 2007

# Survey of PFOS in German livestock

Survey results from 20 of 301 rural districts of Germany

Samples	PFOS		
	(< 2.5 µg/kg)	(2.5 - 5 µg/kg)	(5 - 10 µg/kg)
<b>Animal samples</b>			
Feeder cattle (liver), N = 182	74%	14%	12%
Slaughtered cattle (liver), N = 86	66%	17%	17%
Laying hen (liver), N = 33	94%	6%	0%



## Key points

- Most detections of PFOS in liver were < 2.5 ppb
- Concentrations of PFOS in liver are generally much higher than in muscle
- Analytical methods not described
- Data not published in peer reviewed literature

Reference: S. Effkeman, 2008b

# **Monitoring of PFOA and PFOS in air and water**

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## ***PFOA and PFOS in ambient air***

## ***PFOA and PFOS in water***

- Air
- Surface water
- Oceans
- Wastewater
- Drinking water

# PFOA and PFOS in ambient air

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Location	Mean concentration (pg/m <sup>3</sup> ) *	
	PFOA	PFOS
<u>Rural</u>		
Kjeller, Norway	1.5	1
Mace Head, Ireland	8.9	< 1.8
<u>Marine air</u>		
Near Europe	1.2	1.4
Near Africa	< 0.5	0.5
<u>Urban</u>		
Albany, NY	5.2	2.3
Oyamazaki, Japan	263	5.2
Fukuchiyama, Japan	15.2	2.2
Moriaoka, Japan	2	0.7
Manchester, UK	15.7, 240	46, 7.1
<u>Adjacent to manufacturing</u>		
Parkersburg, WV (fenceline)	10,000 - 75,900	--
Parkersburg, WV (downwind)	10 - 10,000	--

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\* Includes gas and particle phases

Compilation source: ATSDR, 2009

# PFOA and PFOS in surface water

Location	Mean concentration (ug/L)		Reference
	PFOA	PFOS	
<u>USA</u>			
California	0.010 - 0.19	0.020 - 0.19	Larabee and Reinhard, 2008
North Carolina	0.29	0.13	Nakayama et al., 2007
Kentucky	0.022 - 0.33	0.007 - 0.15	Loganathan et al., 2007
Georgia	0.001 - 0.23	0.0018 - 0.022	Loganathan et al., 2007
<u>Japan</u>			
Osaka	0.0052 - 0.092	0.00026 - 0.022	Takagi et al., 2008
Yodo River	0.0042 - 2.60	0.0004 - 0.12	Lein et al., 2008
Tsurumi River	0.013 - 0.016	0.18	Zushi et al., 2008
Kyoto	0.0079 - 0.11	<0.0052 - 0.010	Senthilkumar et al., 2007
Other	0.0001 - 0.46	0.00024 - 0.037	Saito et al., 2004
<u>Italy</u>			
Lake Maggiore	0.003	0.009	Loos et al., 2007
River Po	0.060 - 1.30	0.010	Loos et al., 2008
South Korea	0.0009 - 0.062	0.0024 - 0.65	Rostkowski et al., 2006
Germany	0.0007 - 0.25	0.001 - 0.20	Skutlarek et al., 2006
<u>United Kingdom</u>			
Env Agency GW	<0.10 - 0.60	< 0.10 - 6.30	Env Agency, 2007
Env Agency SW	< 0.10 - 0.34	< 0.10 - 14.5	Env Agency, 2007
Env Agency TRBM	< 0.10 - 2.00	< 0.10 - 33.9	Env Agency, 2007
WRc	< 0.024 - 0.37	< 0.011 - 0.21	Atkinson et al., 2006
<u>China</u>			
Pearl River	0.00085 - 0.013	0.001 - 0.099	So et al., 2007
Yangtze River	0.002 - 0.26	< 0.000001 - 0.014	So et al., 2007

References summarized in ATSDR, 2009

# PFOA in surface water

Study	Location	PFOA (ug/L)
<b>Freshwater</b>		
2001 Multi-city study	6 cities in USA	< 0.0075 - 0.083
2002 Hansen et al	Tennessee River	< 0.025
2002 Moody et al	Etobicoke Creek, Canada	< LOQ - 0.033
2004 Boulanger et al	Lake Erie, Lake Ontario	0.027 - 0.050
2005 Simcik and Dorweiler	Lake Michigan	0.003 - 0.0034
2005 Simcik and Dorweiler	Lake Superior, Voyageurs NP	0.0001 - 0.0007
2005 Simcik and Dorweiler	Urban lakes and rivers in MN	0.0005 - 0.019
2006 Pascagoula baseline study	Rivers and bayous in MS	< 0.013
2006 Sinclair et al	Surface waters in NY	< 0.0005 - 0.0074
2007 Davis et al	Ohio River	< 0.010
2008 Konwick et al	Rivers in GA	0.003 - 0.032
2008 Konwick et al	Ponds, streams in GA	0.050 - 0.054
2008 Plumlee et al	Streams in CA	0.008 - 0.036
<b>Summary:</b>		< LOQ - 0.083
<b>Freshwater impacted by a point source</b>		
2002 Hansen et al (2002)	Tennessee River	< 0.025 - 0.60
2002 Moody et al	Etobicoke Creek, Canada	< LOQ - 10.6
2008 DuPont	Ohio River	0.50 - 4.50
2008 Konwick et al	Rivers in GA	0.25 - 1.15
2008 Konwick et al	Ponds, streams in GA	0.10 - 0.30
<b>Summary:</b>		< LOQ - 10.6

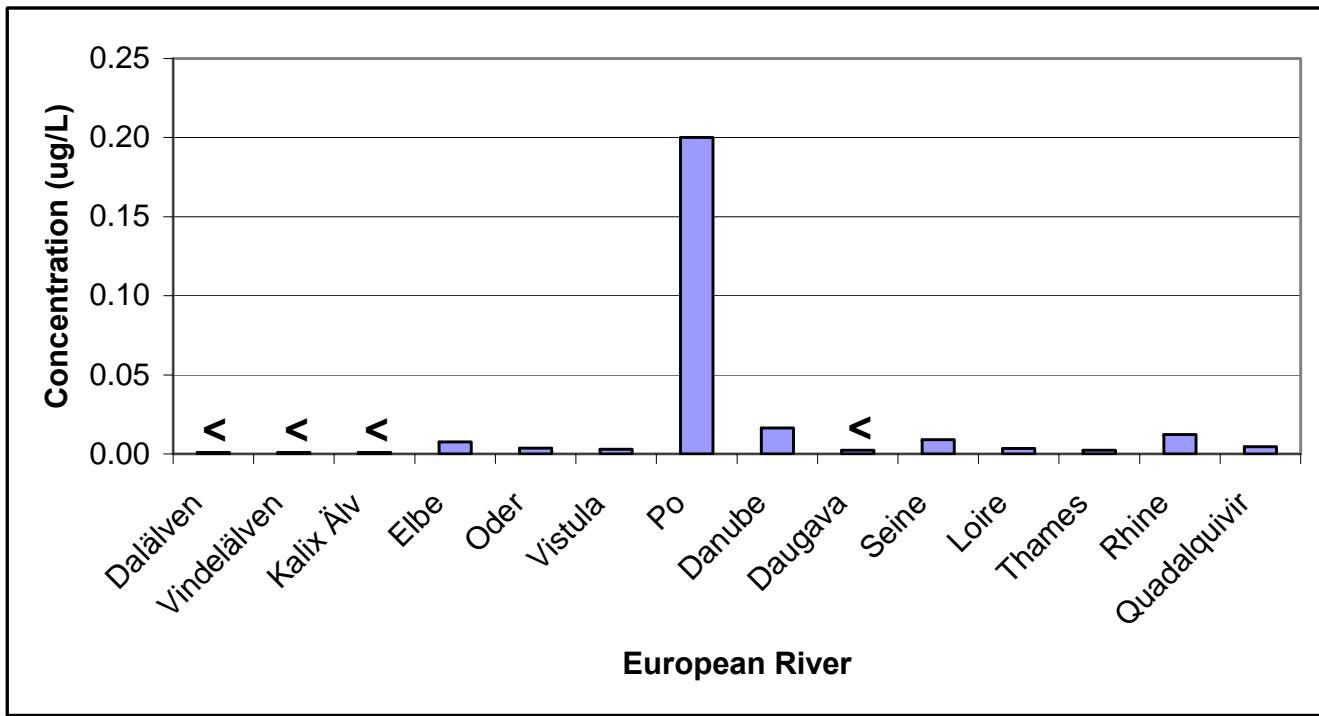
# PFOA in surface water (continued)

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	Study	Location	PFOA (ug/L)
<b>Freshwater</b>			
2004	Kallenborn et al	Finland, seawater	0.004 - 0.006
2004	Kallenborn et al	Denmark, seawater	0.006 - 0.008
2004	Kallenborn et al	Iceland, seawater	0.004
2004	Kallenborn et al	Faroe Islands, seawater	0.004 - 0.007
2004	Kallenborn et al	Lake in Norway	0.005 - 0.008
2006	Skutlarek et al	Rhine River and tributaries	< 0.002 - 0.048
2007	McLachlan et al	13 rivers in Europe	< 0.0007 - 0.025
			<b>Summary:</b> < 0.0007 - 0.048
<b>Freshwater impacted by a point source</b>			
2006	Skutlarek et al	Ruhr River and tributaries	< 0.002 - 3.64
2006	Skutlarek et al	Moehne River and tributaries	< 0.002 - 33.9
2007	McLachlan et al	Po River, Italy	0.20
2007	Environment Agency, UK	Streams and rivers in UK	0.10 - 2.00
			<b>Summary:</b> < 0.002 - 33.9

---

# PFOA in surface water (continued)



Reference: McLachlan et al., 2007

# PFOA and PFOS in oceans

Study	Location	PFOA (ng/L)	PFOS (ng/L)
<b>Ocean monitoring</b>			
2005 Yamashita et al.	{ N Atlantic Ocean Mid Atlantic Ocean W Pacific Ocean Cent to E Pacific Ocean	0.160 - 0.338 0.100 - 0.439 0.136 - 0.142 0.015 - 0.062	0.009 - 0.036 0.037 - 0.073 0.054 - 0.078 0.001 - 0.020
2007 Theobald et al.	N to S Atlantic Ocean	< 0.017 - 0.090	< 0.014 - 0.170
2008 Yamashita et al.	S Pacific Ocean	< 0.005 - 0.011	< 0.005 - 0.011
2008 Wei et al.	{ Cent to S Pacific Ocean Indian Ocean Antarctic Ocean	< 0.005 - 0.007 < 0.005 - 0.011 < 0.005	< 0.005 - 0.021 < 0.005 - 0.009 0.005 - 0.023
2009 Ahrens et al.	{ N Atlantic Ocean Mid Atlantic Ocean S Atlantic Ocean	< 0.004 - 0.229 < 0.004 - 0.087 < 0.004	< 0.010 - 0.291 < 0.010 - 0.060 < 0.010
<b>Summary:</b>		< 0.004 - 0.439	0.001 - 0.291



*Note: Concentrations are in ng/L*

# Municipal Wastewater Treatment of PFOA and PFOS

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Location	Number WWTPs	Sample	PFOA (ug/L)	PFOS (ug/L)	Reference
<b><i>Municipal wastewater, USA</i></b>					
Georgia, rural	1	Influent	0.002 - 0.050	0.003 - 0.008	Loganathan et al., 2007
		Effluent	0.001 - 0.033	0.003 - 0.008	
Kentucky, urban	1	Influent	0.022 - 0.18	0.007 - 0.016	Loganathan et al., 2007
		Effluent	0.12 - 0.18	0.008 - 0.028	
Iowa, urban	1	Influent	> 0.004 (est)	> 0.40 (est)	Boulanger et al., 2005
		Effluent	0.022	0.026	
Pacific NW, urban	1	Influent	0.015	0.015	Schultz et al., 2006
		Effluent	0.011	0.018	
New York, urban	2	Effluent	0.13 - 0.24	0.006 - 0.031	Sinclair et al., 2006
<b><i>Municipal wastewater, Europe and Asia</i></b>					
Singapore, urban	1	Influent	0.013 - 0.082	0.007 - 0.019	Yu et al., 2009
		Effluent	0.016 - 0.15	0.005 - 0.016	
Japan, urban	5	Influent	0.014 - 0.041	0.014 - 0.066	Murakami et al., 2009
		Effluent	0.010 - 0.068	0.043 - 0.11	
Germany, urban	2	Influent	0.002 - 0.004	<0.001 - 0.033	Becker et al., 2008
		Effluent	0.006 - 0.011	0.002 - 0.008	
Germany, urban	6	Effluent	0.012 - 0.069	< 0.0001 - 0.006	Ahrens et al., 2009
Austria, urban	21	Effluent	0.010 - 0.10	0.004 - 0.10	Clara et al., 2008

# Industrial Wastewater Treatment of PFOA and PFOS

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Location	Number WWTPs	Sample	PFOA (ug/L)	PFOS (ug/L)	Reference
<b><i>Industrial wastewater, USA</i></b>					
New York	4	Effluent	0.067 - 0.70	0.004 - 0.009	Sinclair et al., 2006
<b><i>Industrial wastewater, Asia and Europe</i></b>					
Singapore	1	Influent Effluent	0.032 - 0.64 0.077 - 1.06	0.056 - 0.38 0.096 - 0.46	Yu et al., 2009
Japan	1	Influent Effluent	0.028 0.066	0.34 0.64	Murakami et al., 2009
Austria	2	Effluent	0.16 - 0.22	0.20 - 0.34	Clara et al., 2008
Germany	2	Influent Effluent	0.024 - 0.093 0.018 - 0.25	< 0.001 - 0.085 0.009 - 0.20	Becker et al., 2009
Germany	3	Effluent	0.017 - 0.078	0.005 - 0.082	Ahrens et al., 2009
<b><i>Solid waste concentrations</i></b>			(ug/g dw)	(ug/g dw)	
Georgia		Incinerator ash	0.007 - 0.035	< 0.003 - 0.050	Loganathan et al., 2007
Kentucky		Sludge	0.008 - 0.22	0.008 - 0.11	Loganathan et al., 2007
Singapore		Sludge	0.006 - 0.013	0.009 - 0.025	Yu et al., 2009



# PFOA and PFOS in drinking water with identified point sources

Location	Drinking water source	Mean concentration (ug/L) PFOA	Mean concentration (ug/L) PFOS	Reference
<u>Washington, WV</u>				
Private drinking water wells	groundwater	1.55 - 7.20	--	
Public water supply (1 mi downstream)	groundwater	5.60	--	
Public water supply (18 mi downstream)	bank filtration of Ohio R.	0.057	--	
Public water supply (45 mi downstream)	bank filtration of Ohio R.	0.025	--	DuPont, 2009
<u>Oakdale, MN</u>				
Public water supply wells	groundwater	0.51 - 0.83	0.51 - 0.85	3M, 2008-2009
<u>Ruhr area of Germany</u>				
Neheim (highest concentration)	bank filtration of Möhne R.	0.52	0.005	
Wickede (~12 km downstream)	bank filtration of Ruhr R.	0.21	<0.002	
Schwerte (~28 km downstream)	bank filtration of Ruhr R.	0.15	0.013	
Hagen (~44 km downstream)	bank filtration of Ruhr R.	0.034	0.022	Skutlarek et al., 2006



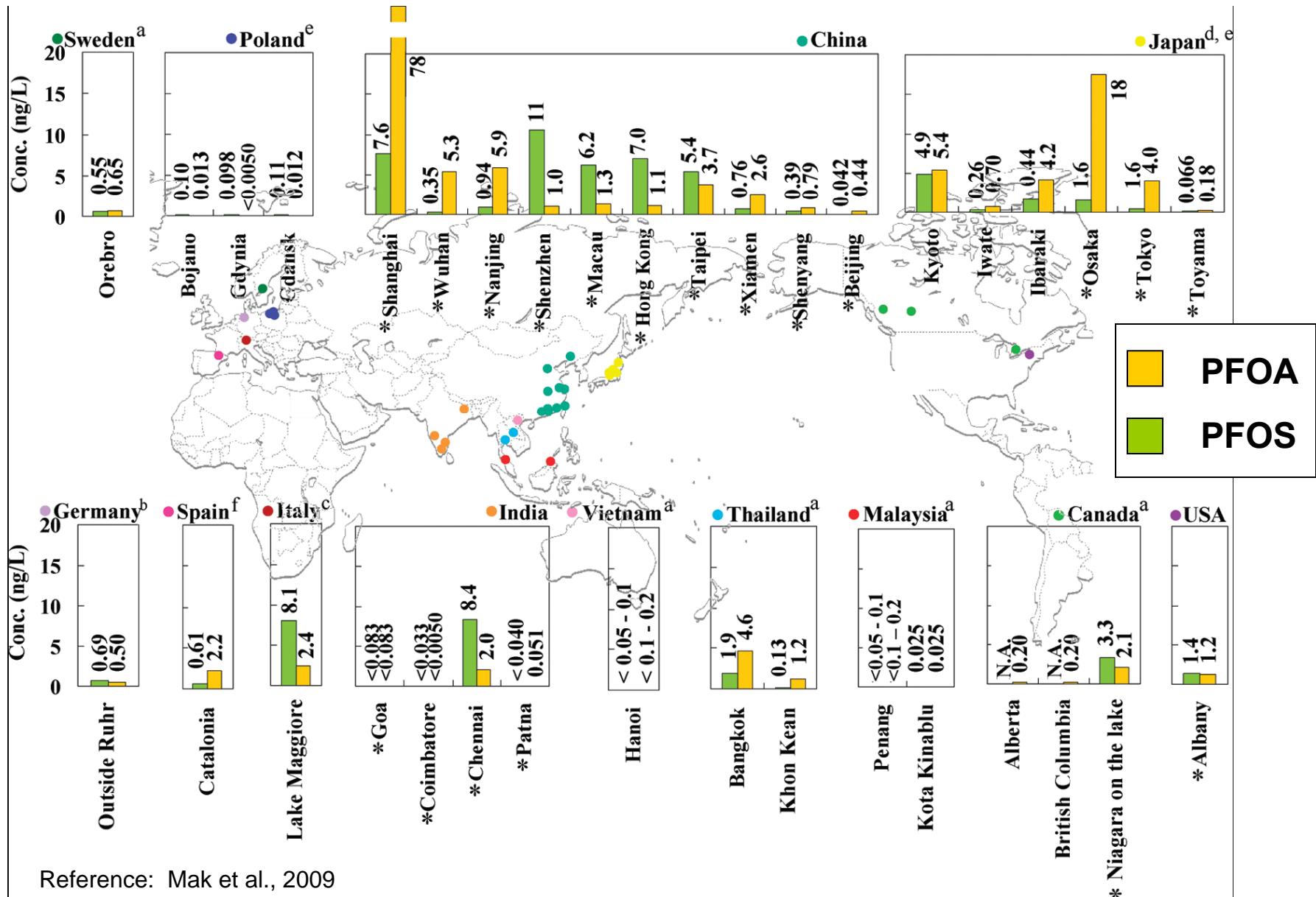
# PFOA and PFOS in drinking water in USA

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Location	Drinking water source	Mean concentration (ug/L)		Reference
		PFOA	PFOS	
New Jersey PWS	groundwater	< 0.010 - 0.140	--	Post et al., 2009
New Jersey PWS	surface water	< 0.004 - 0.039	--	
Decatur, AL	surface water	--	< 0.0025	3M, 2001
Cleveland, TN	surface water	--	< 0.0025	
Mobile, AL	surface water	--	< 0.0025	3M, 2001
Columbus, GA	surface water	--	0.053 - 0.063	
Pensacola, FL	groundwater	--	< 0.0025 - 0.047	3M, 2006, 2007,2008
Port St. Lucie, FL	groundwater	--	< 0.0025	
Decatur WTP, AL	surface water	ND	ND	3M, 2006, 2007,2008
Morgan / Lawrence Co. WTP, AL	surface water	0.043 - 0.160	0.036 - 0.104	
Muscle Shoals WTP, AL	surface water	0.027 - 0.043	ND - 0.044	
Florence WTP, AL	surface water	0.025 - 0.043	ND - 0.044	
Sheffield WTP, AL	surface water	0.029 - 0.042	ND - 0.044	

# Global monitoring of PFOA and PFOS in drinking water

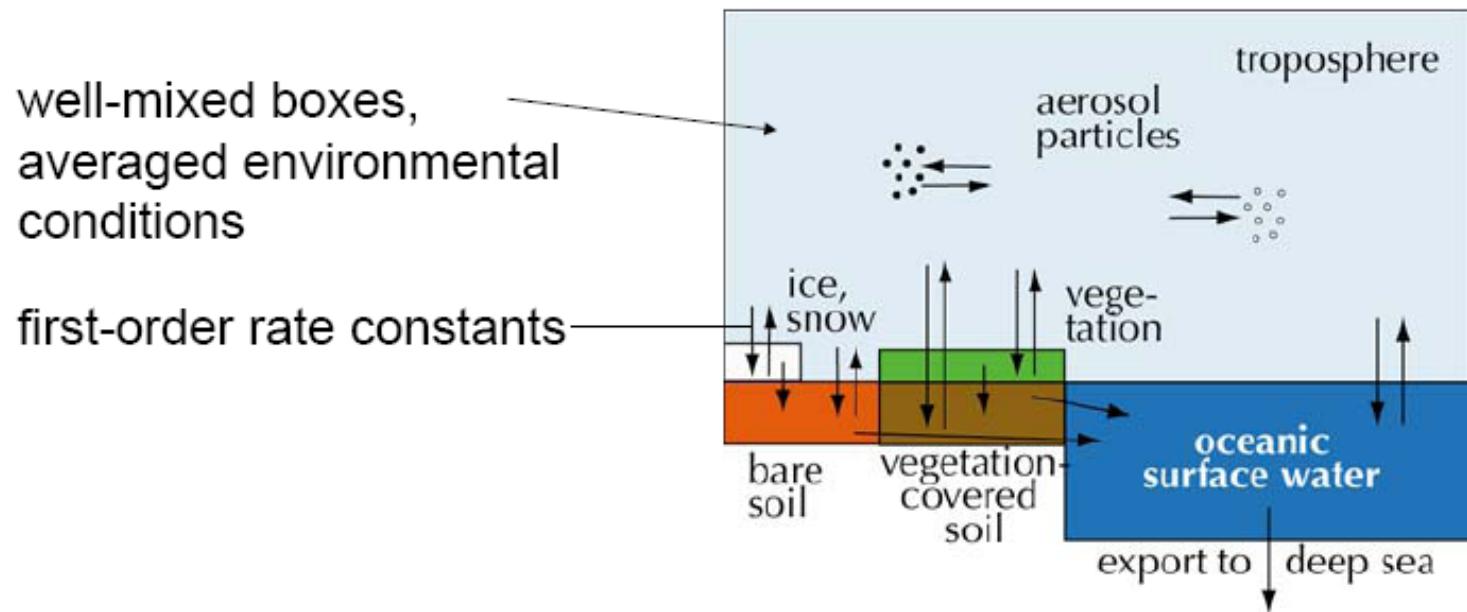
(Note: concentrations are in ng/L)



# Environmental modeling approaches for PFOA and PFOS

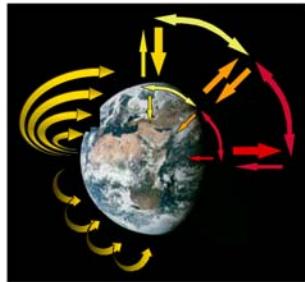
## *Multimedia modeling of soil, air and water*

- Convenient framework for evaluation of environmental concentrations of persistent chemicals
- Appropriate scale is generally large areas over extended periods of time (determined by mixing assumptions)



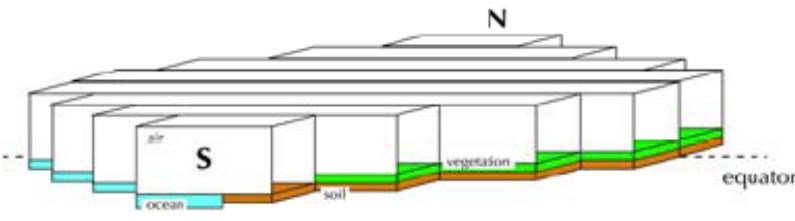
# Examples of environmental modeling of PFOA and PFOS

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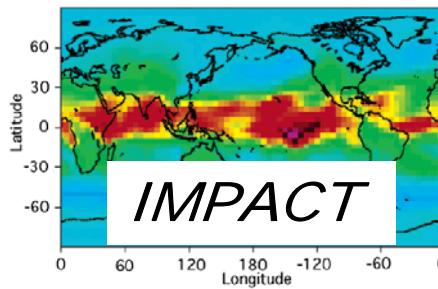
## Globo-POP and BETR

- Applied to C8-C13 and precursors
- 10 zones → 288 zones across earth
- Publications by Armitage et al. 2006 and 2009, Wania et al. 2007



## CLiMoChem

- Applied to PFOA, PFOS and precursors
- Can handle multiple chemicals
- Publications by Schenker et al. 2008 and Armitage et al. 2009

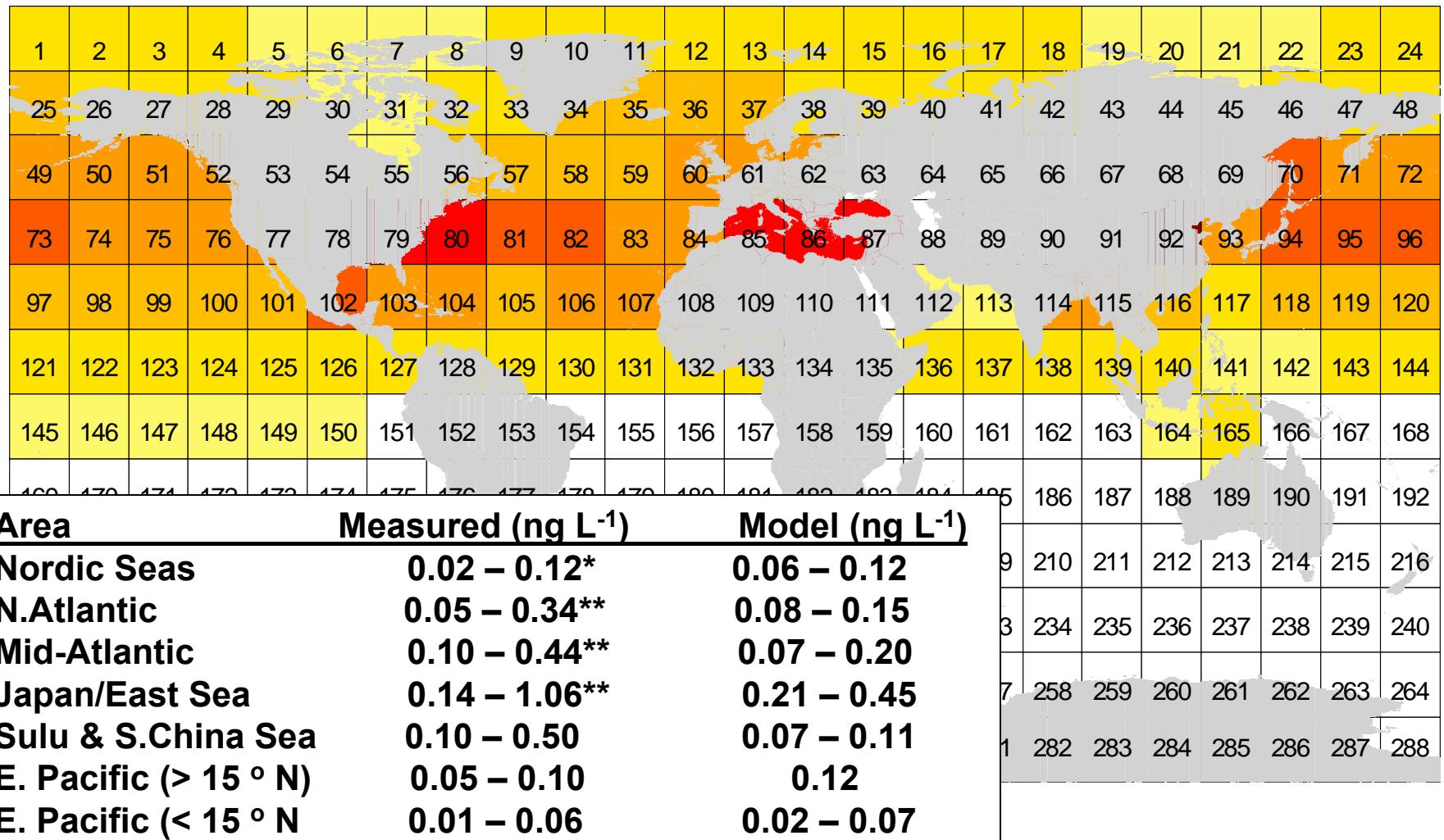


**CAMx** Ozone  
Particulates  
Toxics

## Atmospheric modeling

- IMPACT and CAMx applied to FTOH → PFCAs
- Complex, computationally intensive 3D models
- Publications by Wallington et al. 2005 and Yarwood et al. 2007

# Example of BETR global modeling of PFO(A)



References: Armitage et al., 2009; \* Theobald et al., 2007; \*\* Yamashita et al., 2005, 2007

# Issues with modeling PFOA, PFOS and precursors

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- Simulation **scale**

Most useful when applied to large areas (continental / global) over extended periods of time

- Simulation of **ionizing compounds**

For PFO(A), need to account for both PFO- and PFOA

- **Uncertainty** in physical / chemical properties

For typical POP chemicals (e.g. PCBs), partition coefficients are generally well known and uncertainty exists in degradation rates

PFOA and PFOS are both environmentally stable. Uncertainty exists primarily in physical-chemical data, partitioning behavior and formation kinetics from precursors. Model results will continue to improve as additional experimental values are published.